

Introduction to Differentiable Probabilistic Models

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S&P Global

July 25, 2019

Primer: Standard Machine Learning

- Usually, we are given a set $\mathcal{D} = \{X, y\}$

$$X = \begin{bmatrix} x_{11} & x_{12} & \dots & x_{1m} \\ x_{21} & x_{22} & \dots & x_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \dots & x_{nm} \end{bmatrix} \quad y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

where X is our data matrix, and y are our labels.

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where X is our data matrix, and y are our labels.

- Attempt to fit a model f parameterized by θ with respect to an objective function \mathcal{L}

$$\theta^* = \operatorname{argmin}_{\theta} \mathcal{L}(f(X; \theta), y)$$

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- ▶ Consider our model is a probability distribution Q
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- ▶ Examples:
 - ▶ Classification: Fitting two multinomial distributions
 - ▶ Regression: Fitting a Normal centered around the line of best fit

How do we "fit" Distributions?

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- ▶ This "distance" is known as the divergence between the true distribution P and the learned distribution Q .

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- ▶ Fitting two distributions implies minimizing their difference, i.e. "distance"
- ▶ This "distance" is known as the divergence between the true distribution P and the learned distribution Q .
- ▶ Divergences must satisfy 2 properties:
 - ▶ $D(P \parallel Q) \geq 0 \quad \forall P, Q \in S$
 - ▶ $D(P \parallel Q) = 0 \iff P = Q$

The Kullback-Leibler Divergence

- ▶ The KL Divergence for distributions P and Q is defined as:

$$D_{KL}(P \parallel Q) = \int_{-\infty}^{\infty} p(x) \log \left(\frac{p(x)}{q(x)} \right) dx$$

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- ▶ But we will come back to this later...

Digression: Monte Carlo Integration

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Algorithm 1 $\mathbb{E}_{x \sim P}[f(x)]$

Expectation of $f(x)$ with respect to P

- 1: $x_1, \dots, x_n \sim P$ independently
 - 2: **return** $\frac{1}{N} \sum_{x_i} f(x_i)$
-

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Digression: KL to Cross-Entropy

$$H(P, Q) = - \sum_{x \in \mathcal{X}} p(x) \log q(x)$$

- If we consider $P(y_i = 1|x_i) = p_i$ and $Q(y_i = 1|x_i) = \sigma(f_\theta(x_i))$:

$$\operatorname{argmin}_{\theta} D_{KL}(P \parallel Q) =$$

$$\operatorname{argmin}_{\theta} - \left[p_i \log \sigma(f_\theta(x_i)) + (1 - p_i) \log(1 - \sigma(f_\theta(x_i))) \right]$$

- This is the Binary Cross-Entropy Loss

Forward KL: Learning a Normal Distribution (Initial)

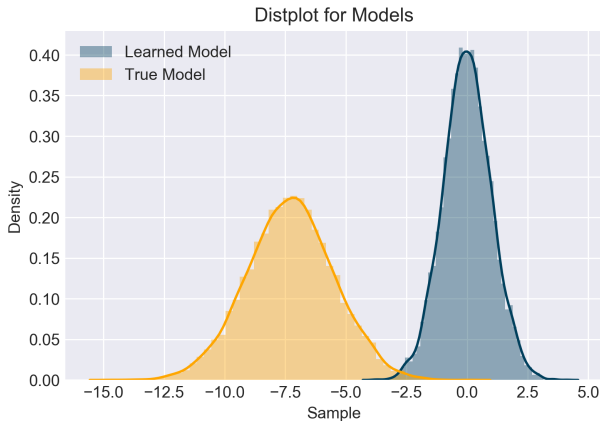


Figure: $P \sim \mathcal{N}(-7.3, 3.2)$, $Q \sim \mathcal{N}(0, 1)$

Forward KL: Learning a Normal Distribution (Results)

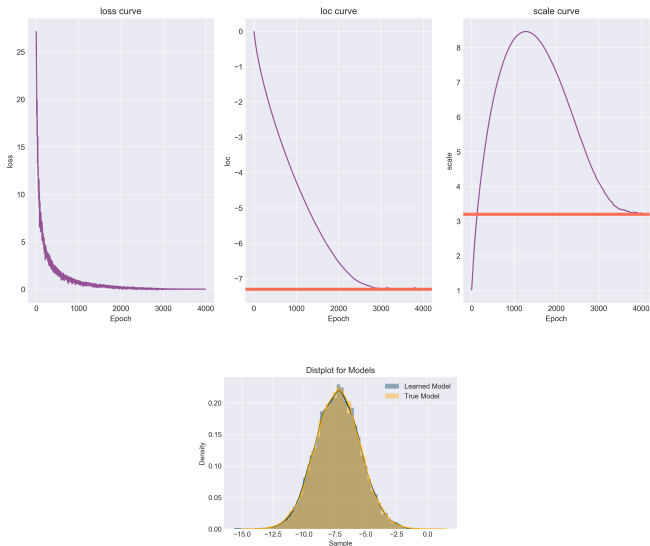


Figure: $P \sim \mathcal{N}(-7.3, 3.2)$, $Q \sim \mathcal{N}(-7.28, 3.24)$

Digression: Gaussian Mixture Models

- ▶ We can build a K multi-modal distribution, with weights π , as follows:

$$z \sim \text{Categorical}(\pi)$$

$$x | z = k \sim \text{Normal}(\mu_k, \sigma_k)$$

- ▶ We can calculate log probabilities by marginalizing out z :

$$\log p(x) = \log \sum_{k=1}^K \underbrace{p(z = k)}_{\text{Categorical}} \cdot \underbrace{p(x | z = k)}_{\text{Normal}}$$

Digression: Mixture Models (Visual)

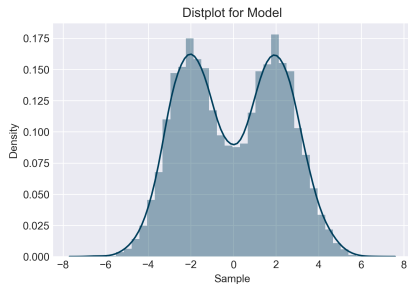


Figure: 2 Mixture Components, Even Weights

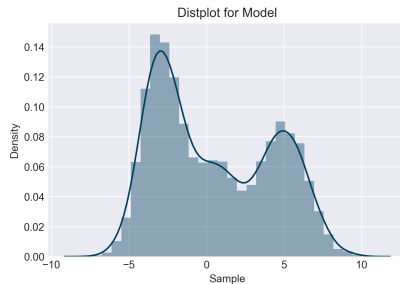


Figure: 3 Mixture Components, Uneven Weights

Forward KL: Learning a Bimodal (Initial)

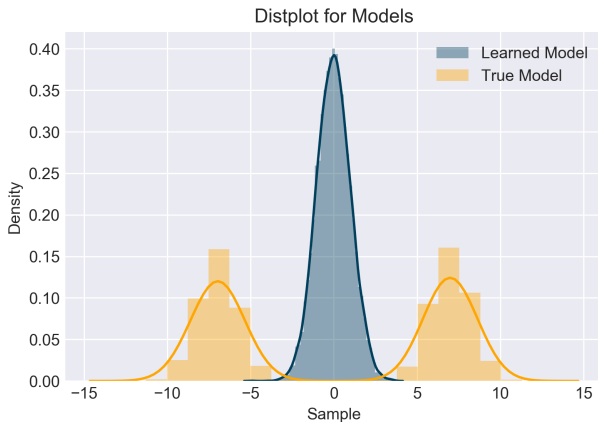


Figure: $P \sim \{\mathcal{N}(-7.3, 1.4), \mathcal{N}(7.3, 1.4)\}$
 $Q \sim \mathcal{N}(0, 1)$

Forward KL: Learning a Bimodal (Results)

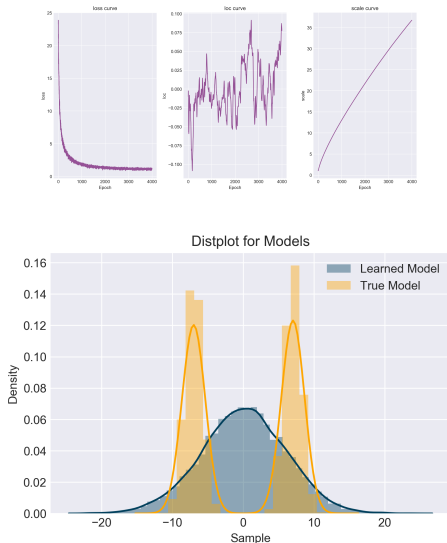


Figure: $Q \sim \mathcal{N}(0.08, 36.76)$

Forward KL: Zero-Avoiding

$$D_{KL}(P \parallel Q) = \int_{-\infty}^{\infty} \overbrace{p(x)}^{\text{Constant}} \log \left(\frac{\overbrace{p(x)}^{\text{Constant}}}{\underbrace{q(x)}_{\text{Variable}}} \right) dx$$

- ▶ $p(x)$ is constant-valued, $q(x)$ is variable
- ▶ If Q does not support P , then we will sample a point that has a low probability with respect to Q

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- ▶ $p(x)$ is constant-valued, $q(x)$ is variable
- ▶ If Q does not support P , then we will sample a point that has a low probability with respect to Q
- ▶ As $q(x) \rightarrow 0$, our loss $D_{KL} \rightarrow \infty$
- ▶ Hence, the optimal solution is for Q to cover P , i.e. averaging

Forward KL: Loss Landscape

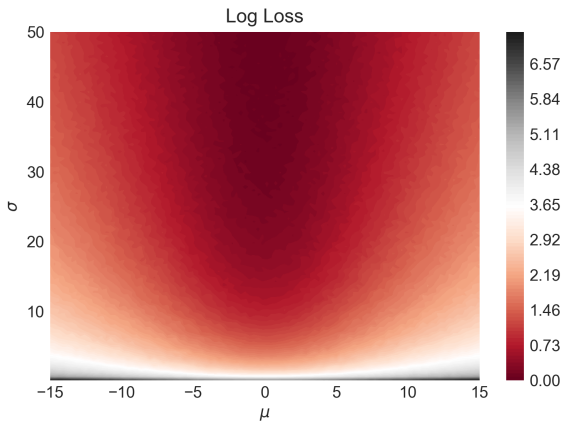


Figure: Loss Landscape for Forward KL Divergence

Directionality: Reverse KL

$$\begin{aligned} D_{KL}(Q \parallel P) &= \int_{-\infty}^{\infty} q(x) \log \left(\frac{q(x)}{p(x)} \right) dx \\ &= \mathbb{E}_{x \sim Q} \left[\log \left(\frac{q(x)}{p(x)} \right) \right] \end{aligned}$$

- ▶ The Reverse KL will sample from Q , and evaluate the log probabilities from P and Q
- ▶ Recall: KL Divergence is not symmetric, and this has drastic implications...

Digression: Differentiable Sampling via the Reparameterization Trick

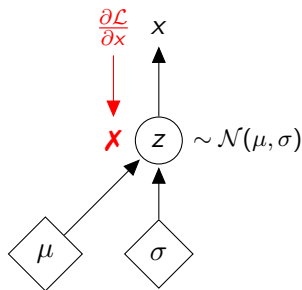


Figure: Original Form

Digression: Differentiable Sampling via the Reparameterization Trick

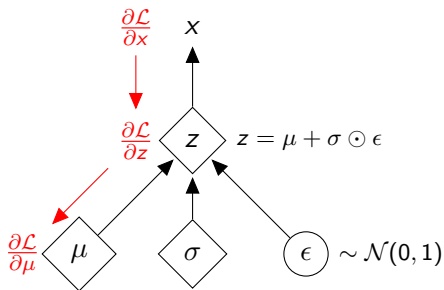


Figure: Reparameterized Version


Digression: Common Reparameterization Tricks

	Reparameterized
$\mathcal{N}(\mu, \sigma)$	$\mu + \sigma \cdot \mathcal{N}(0, 1)$
$\text{Uniform}(a, b)$	$a + (b - a) \cdot \text{Uniform}(0, 1)$
$\text{Exp}(\lambda)$	$\text{Exp}(1)/\lambda$
$\text{Cauchy}(\mu, \gamma)$	$\mu + \gamma \cdot \text{Cauchy}(0, 1)$

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$\text{Laplace}(\mu, b)$	$u \sim \text{Uniform}(-1, 1)$ $\mu - b \cdot \text{sgn}(u) \cdot \ln [1 - u]$

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$\text{Categorical}(\pi)^1$	

¹Can be approximated with Gumbel Softmax

Reverse KL: Learning a Bimodal (Initial)

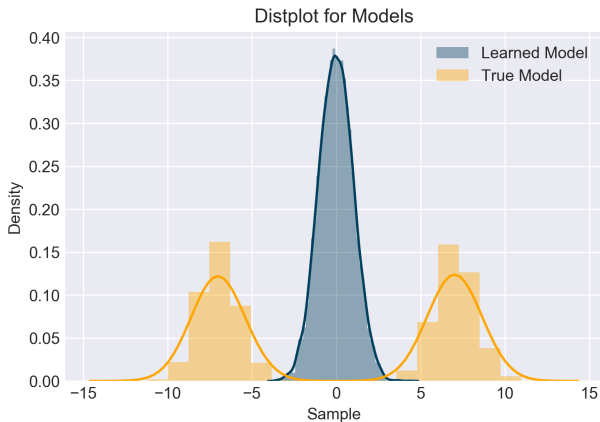


Figure: $P \sim \{\mathcal{N}(-7.3, 1.4), \mathcal{N}(7.3, 1.4)\}$
 $Q \sim \mathcal{N}(0, 1)$

Reverse KL: Learning a Bimodal (Results)

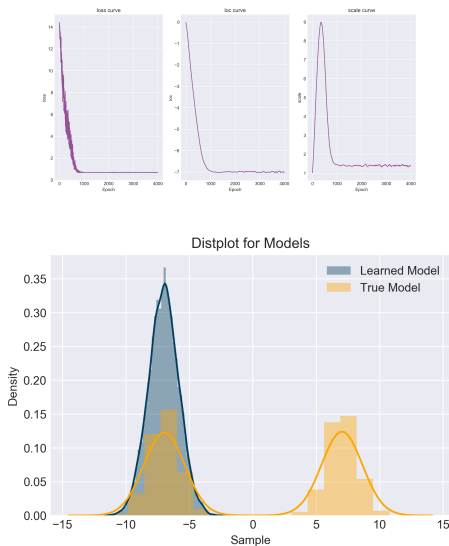


Figure: $Q \sim \mathcal{N}(-7.02, 1.41)$

Reverse KL: Learning a Bimodal Attempt 2 (Results)

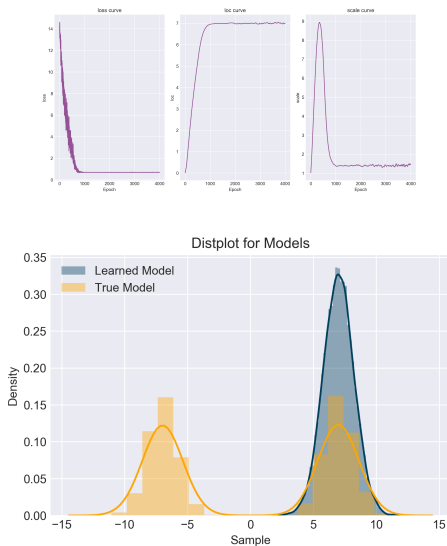


Figure: $Q \sim \mathcal{N}(7.01, 1.46)$

Reverse KL: Zero-Forcing

$$D_{KL}(Q \parallel P) = \int_{-\infty}^{\infty} q(x) \log \left(\frac{q(x)}{p(x)} \right) dx$$

- ▶ Unlike the Forward KL, Reverse KL is Zero-forcing
- ▶ Why? Because we no longer suffer a penalty from $q(x) = 0$
- ▶ However, if $p(x) = 0$, then the optimal value for $q(x)$ is 0
- ▶ Result \implies Mode Collapse

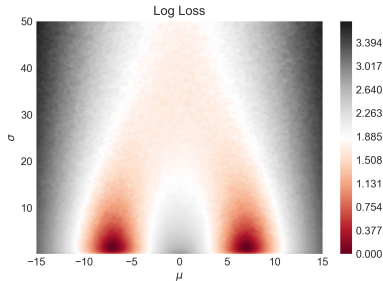


Figure: Loss Landscape for Reverse KL Divergence

Jensen - Shannon Divergence: A Symmetric Divergence

$$\begin{aligned} \text{JSD}(P \parallel Q) &= \frac{1}{2}D_{KL}(P \parallel M) + \frac{1}{2}D_{KL}(Q \parallel M) \\ M &= \frac{1}{2}(P + Q) \end{aligned}$$

- ▶ The JS Divergence is a symmetrized version of the KL Divergence
- ▶ M is the average of distributions P and Q , and can be represented as a Mixture Model

Jensen - Shannon Divergence: Bimodal (Initial)

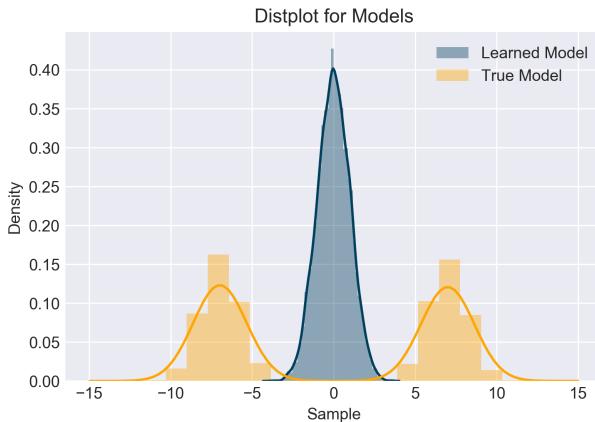


Figure: $P \sim \{\mathcal{N}(-7.3, 1.4), \mathcal{N}(7.3, 1.4)\}$
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Jensen - Shannon Divergence: Bimodal (Result)

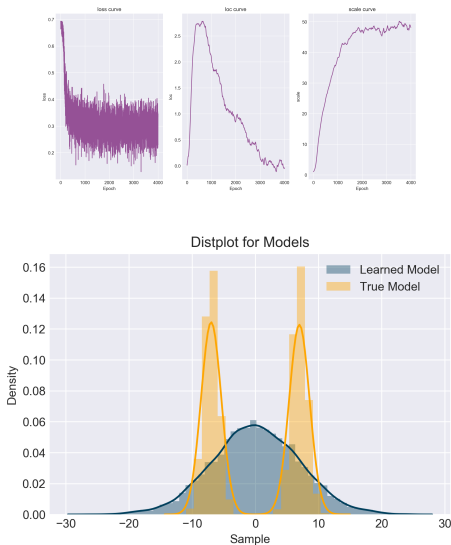


Figure: $Q \sim \mathcal{N}(-0.04, 48.20)$

Jensen - Shannon Divergence: Right Shift (Attempt 2)

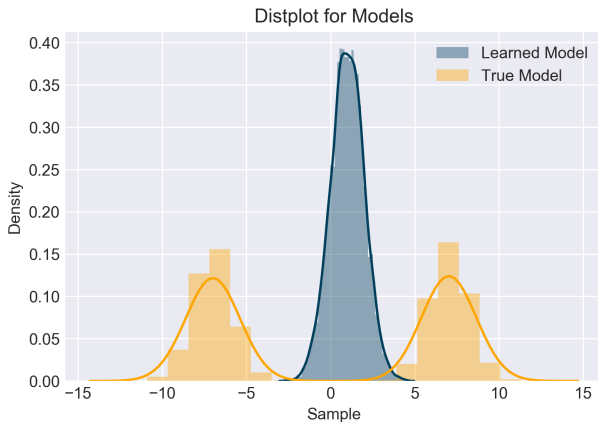


Figure: $P \sim \{\mathcal{N}(-7.3, 1.4), \mathcal{N}(7.3, 1.4)\}$
 $Q \sim \mathcal{N}(1, 1)$

Jensen - Shannon Divergence: Right Shift (Result)

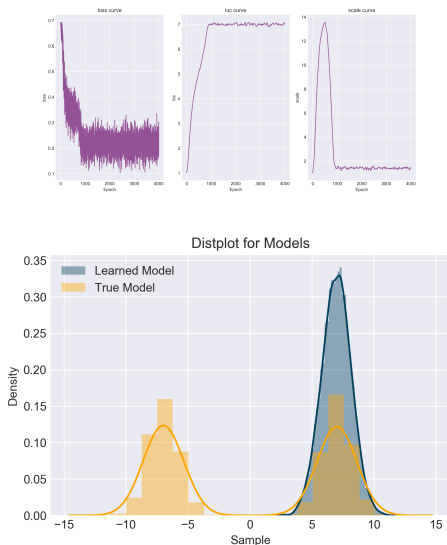


Figure: $Q \sim \mathcal{N}(6.99, 1.43)$

Jensen - Shannon Divergence: Left Shift (Attempt 3)

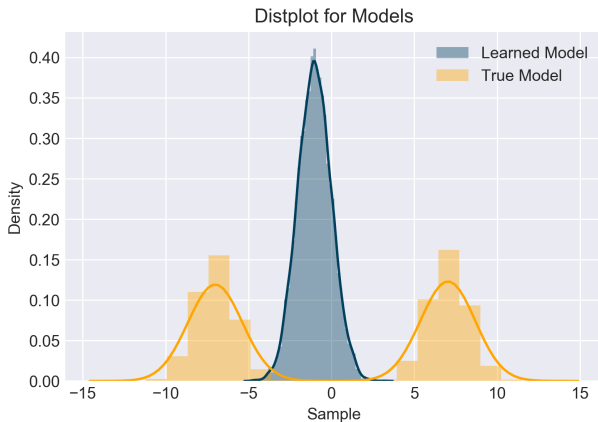


Figure: $P \sim \{\mathcal{N}(-7.3, 1.4), \mathcal{N}(7.3, 1.4)\}$
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Jensen - Shannon Divergence: Left Shift (Result)

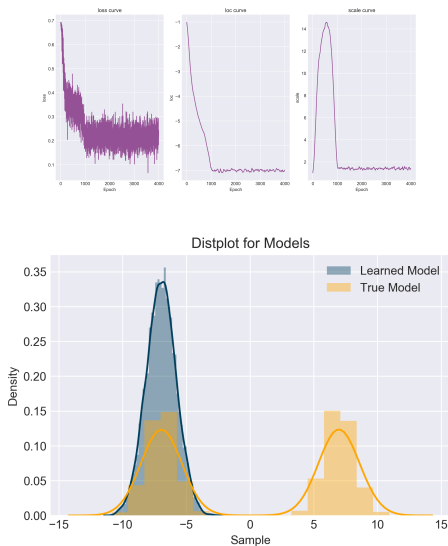


Figure: $Q \sim \mathcal{N}(-6.98, 1.38)$

Jensen - Shannon Divergence Loss

$$\text{JSD}(P \parallel Q) = \frac{1}{2}D_{KL}(P \parallel M) + \frac{1}{2}D_{KL}(Q \parallel M)$$
$$M = \frac{1}{2}(P + Q)$$

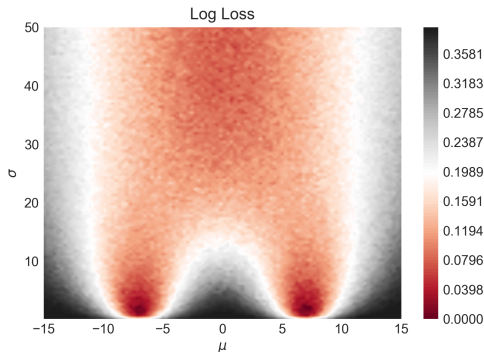


Figure: Loss Landscape for JS Divergence

A Family of Divergences: f -Divergence

- ▶ KL Divergence is a special case of the f -divergence
- ▶ The f -divergence is a family of divergences that can be written as:

$$D_f(P \parallel Q) = \int \overbrace{q(x)}^{\text{Weight}} f \left(\underbrace{\frac{p(x)}{q(x)}}_{\text{Odds Ratio}} \right) dx$$

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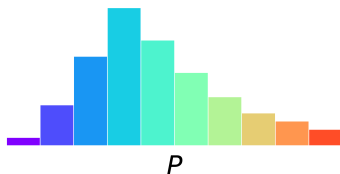
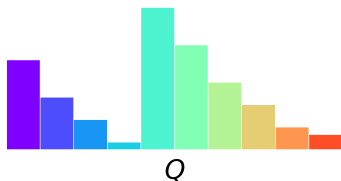
$$D_f(P \parallel Q) = \int \underbrace{q(x)}^{\text{Weight}} \underbrace{f\left(\frac{p(x)}{q(x)}\right)}_{\text{Odds Ratio}} dx$$

Divergence	$f(t)$
Forward KL	$t \log t$
Reverse KL	$-\log t$
Hellinger Distance	$(\sqrt{t} - 1)^2, 2(1 - \sqrt{t})$
Total Variation	$\frac{1}{2} t - 1 $
Pearson χ^2	$(t - 1)^2, t^2 - 1, t^2 - t$
Neyman χ^2 (Reverse Pearson)	$\frac{1}{t} - 1, \frac{1}{t} - t$

Earth Mover's Distance (Wasserstein Distance)

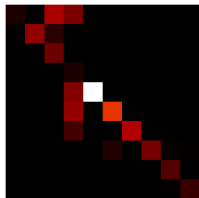
$$\text{EMD}(P, Q) = \inf_{\gamma \in \Pi} \sum_{p, q} \overbrace{\|p - q\|}^{\ell_2 \text{ Norm}} \underbrace{\gamma(p, q)}_{\text{Joint Marginal}}$$

- ▶ $\gamma(p, q)$ states how we distribute the amount of "earth" from one place q over the domain of p , or vice versa
- ▶ EMD is the minimal total amount of work it takes to transform one distribution into the other

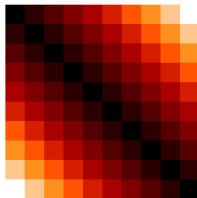


Earth Mover's Distance (Wasserstein Distance)

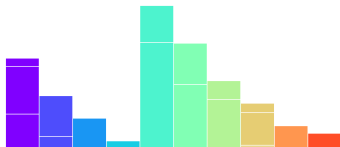
$$\text{EMD}(P, Q) = \inf_{\gamma \in \Pi} \sum_{p, q} \|p - q\| \gamma(p, q)$$



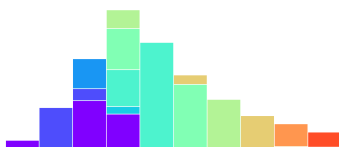
Γ



D



Q



P

Summary of Methods

	P		Q	
	$\log p(x)$	$x \sim P$	$\log q(x)$	$x \sim Q$
Cross-Entropy		✓	✓	
Forward KL	✓	✓	✓	
Reverse KL	✓		✓	✓
JS Divergence	✓	✓	✓	✓
f -Divergence	✓		✓	✓
Wasserstein ²		✓		✓

Practical Uses of Divergences

- ▶ Forward Kullback-Leibler
 - ▶ Maximum Likelihood Estimation
 - ▶ ℓ_2 : Mean Squared Error (Normally Distributed)
 - ▶ ℓ_1 : Mean Absolute Error (Laplace Distributed)
 - ▶ Binary Cross Entropy (Bernoulli Distributed)
 - ▶ Cross Entropy (Multinomially Distributed)
 - ▶ Log-Likelihood Models
 - ▶ PixelCNN
 - ▶ Glow
 - ▶ Variational Autoencoders

Practical Uses of Divergences

- ▶ Reverse Kullback-Leibler
 - ▶ Evidence Lower Bound (ELBO)
- ▶ Jensen-Shannon Divergence
 - ▶ Generative Adversarial Network (Original)
- ▶ Earth Mover's Distance
 - ▶ Wasserstein GAN (WGAN)
- ▶ Pearson χ^2 Divergence
 - ▶ Least Squares GAN (LSGAN)

Potpourri: Advanced Techniques

1. Invertible Transforms
 - ▶ Normalizing Flow Models
2. Expectation–Maximization
3. Variational Inference
 - ▶ ELBO
4. Adversarial Training (Forest of GANs)
5. Markov Chain Monte Carlo
 - ▶ Metropolis-Hastings
 - ▶ Gibbs Sampling
 - ▶ Hamiltonian Monte Carlo
 - ▶ NUTS

Source Code

- ▶ Repo for Differentiable Probabilistic Models
- ▶ Notebook to generate training examples
- ▶ Notebook for EMD
- ▶ \LaTeX source code for presentation

Further Reading

- ▶ Machine Learning: A Probabilistic Perspective by Kevin Murphy
- ▶ Friendly Introduction to Cross-Entropy Loss
- ▶ Categorical Reparameterization with Gumbel Softmax
- ▶ Wasserstein GAN and the Kantorovich-Rubinstein Duality
- ▶ Are all GAN's created Equal?
- ▶ Tutorial on MCMC Methods